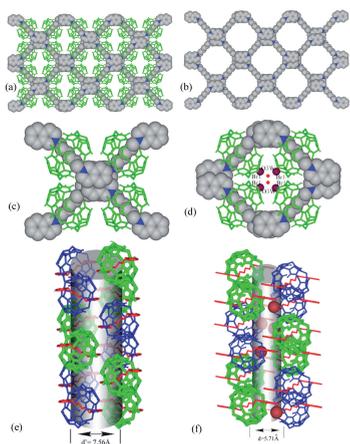


Feng Xue,^b Qian-Jiang Zhu,^b Zhu Tao,^b ^aCSIRO Materials Science and Engineering, P.O. Box 218, Lindfield, NSW 2070, (Australia). ^bKey Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang 550025, People's (Republic of China). ^cLiupanshui Normal College, Guizhou Province, 553004, People's (Republic of China). E-mail: gang.wei@csiro.au or sfxue@gzu.edu.cn

Q[n]-based supramolecular architectures which have intriguing structures or their potential applications in gas storage or absorption, catalysis, and optoelectronics, have been of great interest in the cucurbit(n)urils (Q[n]s) chemistry.[1-4] In present study a bromide salt of 2,2'-(hexane-1,6-diyl) diisoquinolinium (K6) was introduced to construct a novel framework induced by $\pi\cdots\pi$ stacking of 2,2'-(alkylene-1,6-diyl)diisoquinolinium from Q[6]-based pseudo-rotaxanes. ¹H NMR spectra analysis was performed and confirmed the pseudorotaxane interaction model in which the 2,2'-(alkylene-1,6-diyl) diisoquinolinium guest threads into the cavity of Q[6] with the alkyl chain included inside the cavity and the two end isoquinolyl moieties protruding from the two opening portals. The crystal structure of the compound revealed that the assembled framework based on the Q[6]-2,2'-(alkylene-1,6-diyl) diisoquinolinium pseudo-rotaxanes have stoichiometries of $\{(K6)@(Q[6])\}^{2+}\cdot 2Br^{-}\cdot 7(H_2O)$ (1). The compound (1) has a novel three-dimensional framework constructed of two different channels – one containing stacked isoquinolyl moieties from the K6@Q[6] pseudorotaxanes and the other containing the bromide anions (See figure below). Absorption spectrophotometric and fluorescence spectroscopic analyses of the host-guest inclusion complex in aqueous solution found that the complexes were most stable at a host:guest mole ratio of 1:1. At this ratio, the complex has binding constants (K) $\sim 10^6$.



[1] J. Lagona, P. Mukhopadhyay, S. Chakrabarti, L. Isaacs, *Angew. Chem., Int. Ed.*, **2005**, *44*, 4844-4870. [2] X.-L. Ni, J.-X. Lin, Y.-Y. Zheng, W.-S. Wu, Y.-Q. Zhang, S.-F. Xue, Q.-J. Zhu, Z. Tao, A.I. Day, *Cryst. Growth Des.* **2008**, *8*, 3446-3450. [3] J.-P. Zeng, S.-M. Zhang, Y.-Q. Zhang, Z. Tao, Q.-J. Zhu, S.-F. Xue, G. Wei, *Cryst. Growth Des.* **2010**, *10*, 4509-4515. [4] H. Kim, Y. Kim, M. Yoon, S. Lim, S. M. Park, G. Seo, K. Kim, *J. Am. Chem. Soc.* **2010**, *132*, 12200-12202.

Keywords: framework, $\pi\cdots\pi$ stacking, pseudorotaxane

MS49.P23

Acta Cryst. (2011) A67, C541

Study of ZnO nanoparticles thin films deposited by spin-coating
 Alberto Alvarado-García,^a Hector Juarez,^b Mauricio Pacio,^b Godofredo García,^b Rene Perez,^b ^aCINVESTAV-IPN, programa de Nanociencias y Nanotecnología, Av. Instituto Politécnico Nacional # 2508, Col. San Pedro Zacatenco, C.P. 07360, México, D.F. (México). ^bCIDS-BUAP, Benemérita Universidad Autónoma de Puebla, Ciudad Universitaria Avenida San Claudio y 14 Sur, 72570, Puebla, (México). E-mail: jalvarado@cinvestav.mx

Thin films of zinc oxide nanoparticles, were deposited by spin coating method using glass and silicon as substrates. The obtained films were treated only at 100 °C to evaporate the solvent were the

nanoparticles stay after de deposition. The structural characterization was performed using XRD and SEM techniques in order to observe the differences of film deposition between the substrates. The ZnO thin films showed polycrystalline hexagonal structure when silicon was used as substrate and the other one shows a preferential deposition in 002 ZnO plane. UV-Vis characterization was used to analyze the optical transmittance of the thin films.

Keywords: films, ZnO nanoparticles, spin coating

MS49.P24

Acta Cryst. (2011) A67, C541-C542

Crystal Nucleation in X-ray Amorphous Natural Silicates

Yevgeny A. Golubev *Laboratory of Structural and Morphological Crystallography, Institute of Geology of Komi SC of Ural Division of RAS, Syktyvkar (Russia).* E-mail: golubev@geo.komisc.ru

The paper reports on crystal nucleation in natural x-ray amorphous silicates – noble and ordinary opals, volcanic and impact glasses. It is known, that opal is unstable and easy dehydrated for its high solubility in geological conditions. It forms crystalobalite, tridymite and quartz. The transformation occurs under widely known scheme: opal-A – opal-CT – chalcedony – quartz. Usually opals are mixture of amorphous and different degree ordered silica [1-3]. Classical suggestions about structure of noble opals – in regular intervals located spherical particles (size 100 – 500 nm) consisting of small globules in diameter of 10–50 nm, and larger globules are characteristic for opals with crystal structure elements (crystalobalite – tridymite), and in amorphous opals the sizes of primary globules are estimated in 20–50 nm. However in literature experimental data on electron-microscopic observations of internal structure of small particles in opals practically are not presented. Areas in the size of 10–30 nm with ordered atomic lattice as tridymite or crystalobalite crystals which are settling down in a disorder opal matrix in amorphous opals [4], are often observed.

We studied hypergenic noble opal from residual soil (Australia), opal of hydrothermal origin from deposit Raduzhnoe, Primorsky Region, Russia, and also ordinary opal from Spain by HRTEM, AFM and IR-spectroscopy.

By means of AFM images on regular basis packed of classical globular structure of noble opals with average diameter of globules 260 nm have been received. It is known, that opal globules are aggregated from smallest particles, however by means of AFM to us them to distinguish it was not possible. HRTEM images of the Australian opal show fragments of round particles which diameter makes from 4 up to 5 nm. These are primary globular particles which form globules observable by means of AFM.

In the Australian opal of the ordered lattice fringes to reveal it was not observed. HRTEM images show all, that the opal substance is amorphous state which shows characteristic irregular contrast. For comparison, in opal which on X-ray and IR-spectroscopic data can be carried to crystalobalite opal, HRTEM images show continuous amorphous matrix in which are included nanosized areas with crystal ordering. They are chaotically oriented from each other. Lattice distances correspond of crystalobalite. On contours it is shapeless areas though also polygonal forms in some cases are observed. In the given substance we deal mainly not with nanocrystal, and with ordered fragments of a silica network in disordered environment. It is crystal nucleation center.

The similar ordered areas in natural impact glass have been revealed. Fracture surfaces of the impact and volcanic glasses vary the sizes and the form of the isolations connected with glass nanoparticles.

The work is supported by The Program of Presidium RAS n. 17, Scientific School (7198.2010.5), RFBR 11-05-432a.